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ECCES

**A Model for Calculation of Environmental
Consequences from Energy Systems
Predicting Ion Concentrations and Acidification
Effects in Terrestrial Ecosystems**

K. Brodersen, P. B. Mortensen and T. Petersen

**Risø National Laboratory, DK-4000 Roskilde, Denmark
October 1986**

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ECCES - A MODEL FOR CALCULATION OF ENVIRONMENTAL
CONSEQUENCES FROM ENERGY SYSTEMS PREDICTING ION
CONCENTRATIONS AND ACIDIFICATION EFFECTS IN
TERRESTRIAL ECOSYSTEMS

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T. Petersen

Abstract. ECCES is an environmental management model designed to predict environmental impacts from a given energy production scenario in a given geographical area for a period of time. Presently ECCES contains submodels for atmospheric dispersion and deposition of pollutants, soil chemistry and uptake in selected crops. Dispersion is based on a traditional plume model and calculates dispersion of pollutants from many sources (power plants) to counties at Zealand. The soil chemistry model calculates chemical equilibrium between adsorbed and soluble ions in maximum 5 soil layers. CEC is divided between a permanent and a variable cation exchange capacity. Ion uptake in crops is proportional to the equilibrium concentration in the soil water.

ECCES is implemented in FORTRAN-77. Inputs are from plant, soil, and crop libraries. Output are prints or datafiles transferable to an independent plot program. Scenario calculations illustrate the capabilities of the program, and sensitivity of some important parameters.

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1. INTRODUCTION

Increased rainfall acidity and airborne pollution over Northern and Central Europe and also in other places is causing concern about environmental impact on different ecosystem and demand for tools for administrators and politicians in making decisions.

This paper describes the state of development of the ECCES program system which is designed to predict environmental impacts from a given energy production scenario in a given geographical area for a period of time.

The ECCES model is developed in collaboration between the chemistry and the energy technology departments at Risø National Laboratory. It is a part of a general effort to model the environmental effects of energy production. The project is financed partly by a research grant from the Danish Ministry of Energy and is conducted under guidance from a group with representatives from the Danish Environmental Protection Agency and the Danish Utilities.

In its ideal form, the model should be able to predict environmental impacts in a very broad sense such as human health effects, impacts on agricultural production and forests, and detrimental effects on man made structure (corrosion). It is realized that such a model have to contain submodels describing processes of which knowledge in some cases is controversial, sparse or even non-existent.

All impacts will be calculated based on values averaged over one or several months for concentrations of pollutants in the environment and doses experienced by human beings. Thus high concentration events will not be directly included.

In the present stage of the project a model which follows the transport and transformation of airborne pollution from the source via dispersion in the atmosphere and deposition on the ground, to uptake in selected crops, has been developed.

Sources for pollution may be point sources such as power plants or area sources such as built up areas with individual heating. As pollutants are chosen, in a first example, Cd and SO₂, the latter representing a pollutant undergoing chemical reaction in the atmosphere. The geographical area (see Fig. 1) to be considered in the scenario will be the island of Zealand (on which Copenhagen is situated). The scenario is defined by giving the emission and position of the pollution sources on Zealand and a description of those areas within Zealand in which the environmental impacts should be studied. A description of an area includes data as sizes of areas in which crops are grown, sizes of built up areas, data for soil properties etc.

The model presently contains submodels for atmospheric dispersion and deposition, soil chemistry, uptake in selected crops, and a main program which has a description of the geographical area and positions of sources in it and which can handle data transfer between the submodels.

The dispersion model has been developed to calculate the concentrations in air and the deposition on ground surface of pollutants emitted from chimneys.

The model is restricted to distances not over ~ 100 km and to time intervals not shorter than ~ 1 month.

The soil chemistry model is a compartment model that calculates long-term changes in ion concentration in the upper soil layers as influenced by acid precipitation or by deposition of nutrients or polluting materials.

A set of equations are described which in a simplified manner describe the hydrology and the chemical reactions taking place when rain water is percolating through a top soil layer or a

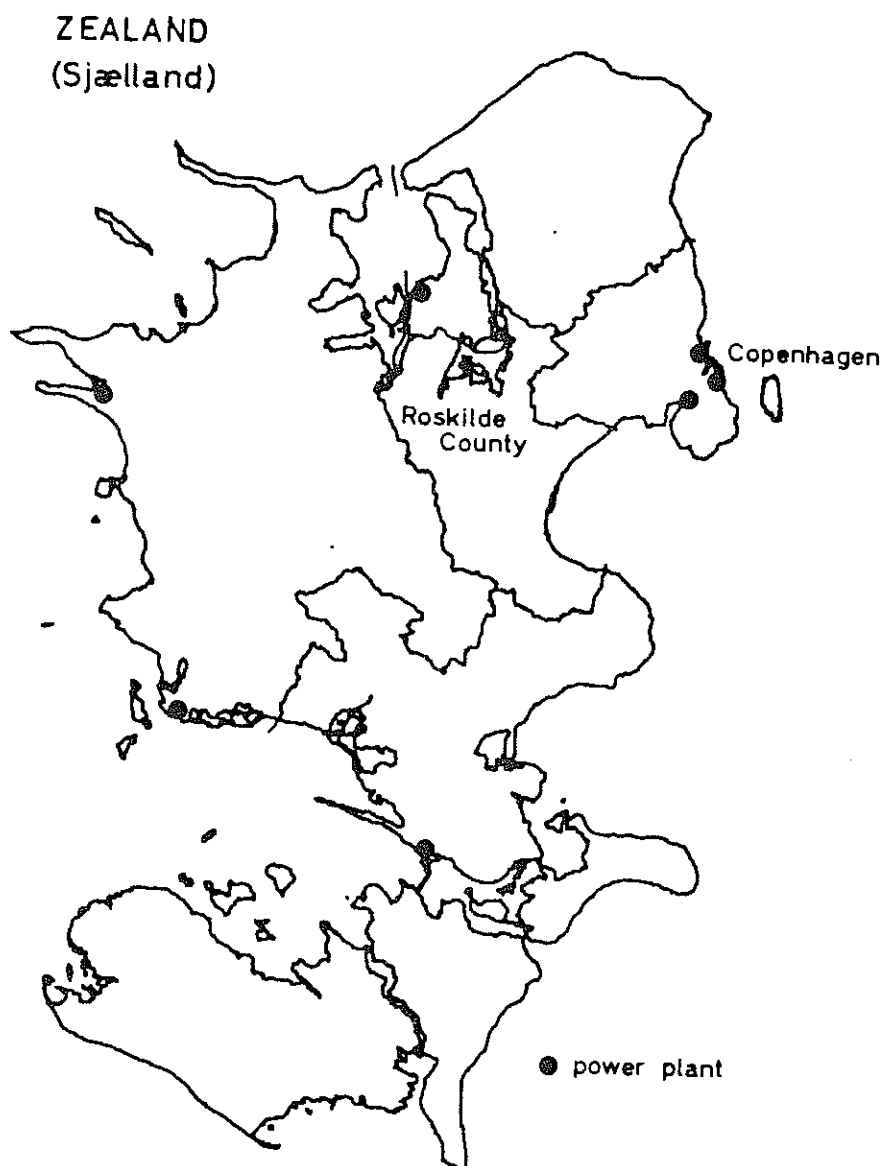


Fig. 1. Geographical area used in scenario.

succession of soil layers below each other. Ion exchange reactions as well as the carbon dioxide equilibria and the precipitation or dissolution of lime or gypsum are taken into account.

The result of the model calculation is the time development of the soil pore water composition which then may serve as basis for the calculation of uptake of polluting materials in plants. The crop model calculates the uptake of nutrients and pollutants from the interstitial water of the soil and deposition of pollutants from the air to the crop surface. Proton release or consumption as a consequence of ion uptake from the soil water is estimated.

The calculations shown in the following intend to demonstrate some phenomena concerning the soil chemistry and crop model and to show the sensitivity of the results to some of the key parameters of the models. Results of scenario calculation where all the submodels are brought into play is shown.

Though the main body of data for all the calculations is chosen as realistic as possible the model must be regarded a preliminary one due to simplifying assumptions and uncertainty about some data.

The model has been implemented in a FORTRAN-77 program on the B7800 computer at Risø National Laboratory. The program consists of about 12800 lines of code, where a little more than half are real FORTRAN-statements, and the rest are comments. The submodels can be run independently.

Input to the program can be divided into three parts:

1. Scenario-defining information: areas, power plants, cities, crops, soil types and pollutants. Start time, simulation time and time step.
2. Model-defining information: which models are to be used. Output options for print and plot.
3. Dynamic information: load factors for each time step with the dispersion model.

There is a large number of output possibilities so nearly all combinations can be made. This is especially useful for testing purposes.

2. MODEL STRUCTURE AND THEORY

2.1. General description

As indicated in the introduction airborne pollution may be followed from sources (power plants etc.) to uptake in plants. The program structure is shown in Fig. 2.

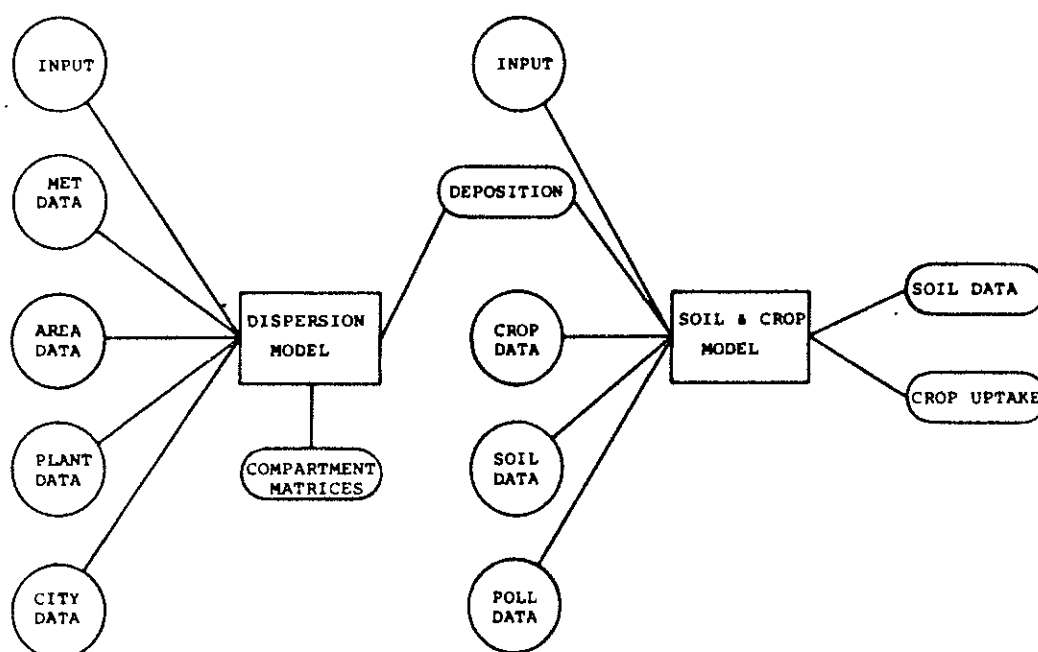


Fig. 2. Program structure.

A key feature of the program is the description of the geographical area under consideration relative to a rectangular coordinate system. The positions of sources as well as receptor points are given in this system.

In the time domain the program operates in discrete time steps, typically a year or a fraction of a year. However, each of the submodels may operate with different time steps in the same run as mentioned in more detail later in this paper.

In designing the program structure care has been taken to obtain as large a flexibility as possible. It is intended that program modules for submodels may easily be replaced. During development of the program it is also ensured that most of the submodels shall exist as separate programs.

Thus dispersion calculations alone may be carried out where input are emissions and positions of sources in a geographical area. The results are concentration in air and amount of deposition of pollutants in selected points.

In the same way the soil chemistry and plant models may be run alone to show changes in soil chemistry and uptake in plants when ions and water are added to the surface of the soil.

The dispersion model is able to calculate dispersion of pollutants from a number of sources to a number of recipients. The sources are the point sources: power plants and the area sources: cities and counties (Danish: amt). The actual sources can be selected in a library of plants, cities and areas. The sources are characterised by their coordinates in a cartesian coordinate system and by the source strength (kg/sec) for each pollutant at maximum energy production for each source. For power plants moreover the chimney height is given.

Pollutants which are studied in a scenario, are also chosen by the input. The data for the pollutants: mole weight, valency, decay constants, deposition velocity, etc., are fetched from a pollutant library.

The dynamics in the model are introduced by a loadfactor (0 - 1) for each source. The load factors are given as input, but at present the time step length in the dispersion model is half a year, so only seasonal variation and long term changes in the power production scheme can be modelled.

The recipients of the pollution are the areas, the data of which are also selected from a library of areas. Deposition of

pollutants of an area is calculated as if deposition takes place at the position of the "center of mass" for the area.

Besides the source- and recipient-defining data is a datafile describing the weather through out the scenario. This datafile contains data describing wind direction, velocity etc.

Output from the dispersion model is airconcentration ($\mu\text{g}/\text{m}^3$) and deposition ($\text{g}/\text{m}^2/\text{year}$) of the pollutants. If the pollutants undergo a chemical transformation in the air under the transport, the concentration and deposition are calculated for both the parent and the daughter product.

The soil chemistry model starts where the dispersion model ends, namely with the deposition as input to the model. The soil chemistry model can be used in conjunction with the dispersion model or alone. If it is used alone it is possible to select one or more soil types from a soil type library. The soil type library contains data such as the number of layers, the water capacity for each layer, the ion exchange capacity for each layer, etc. Seven different typical Danish soil types have been defined.

The soil chemistry model alone calculates chemical equilibrium in each soil layer. Pollutants are added to the upper layer either as contained in rain or in fertilizer. The water containing the different ions percolates through the soil layers (maximum 5), and the gradual change of chemical equilibria in the compartments are modelled.

If the soil chemistry is used together with the dispersion model the soil types are not specified. Instead the actual geographical recipient areas in the scenario are simulated and typically these have areas with all soil types. The area library contains information about the area of each soil type (km^2) for the geographical areas. The model calculates the chemical equilibrium for all soil types in the recipient area with supply to the upper layer of rain plus the calculated deposition from the dispersion calculation.

The crop model is the third and last module in the simulation complex and this module demands that the soil chemistry model also is used. It is possible to simulate uptake of ions in different crops and again the actual crop data are selected through the input from a crop library. This library contains information about crops, such as biomass, water uptake, etc. for each month in the year.

The crop model is closely connected to the soil chemistry model, assuming that the ion uptake is proportional to the equilibrium concentrations of the ions in the soil water.

The output from the crop model is concentrations ($\mu\text{g/kg}$) of ions (pollutants) in the harvested crop each year in a given area. These resulting concentrations are summed over the soil types weighed with the soil type areas. Additional output is the pH in the upper soil layer of all the soil types "beneath" the crops.

2.2 Dispersion model

The following gives a qualitative description of the dispersion model in the ECCES program system. The model calculates air concentration and deposition rate of a pollutant, emitted from a chimney and not generated during the transport away from the chimney.

The model assumes a homogeneous distribution of the smoke across the plume. This gives in this context results comparable to the Gaussian dispersion model since averaging over long time intervals makes the concentration in a given horizontal sector homogeneous over the sector and proportional to the probability that the wind is blowing in a direction from the chimney that lies within the sector. Almost the same result is obtained when the Gaussian distribution is averaged over a sector.

In the vertical (z) direction the two distribution functions are a little more different. The present model assumes a vertical

extension of the plume which is $4 \cdot \sigma_z(x)$, where $\sigma_z(x)$ is the vertical dispersion parameter of the Gaussian model.

The distribution within the plume is assumed to be homogeneous, and outside the plume to be zero. As illustrated in Fig. 3 the upper and lower plume fronts will sooner or later reach the inversion layer and the ground surface, respectively. If the distances, where this occur, are denoted x_L and x_S , we can see that the extension of the vertical plume $\Delta z(x)$, is given by

$$\Delta z(x) = \begin{cases} 4 \cdot \sigma_z(x) & \text{if } x < x_{\min} \\ L - H + 2 \cdot \sigma_z(x) & \text{if } x < x_S \text{ and } x_L < x_S \\ H + 2 \cdot \sigma_z(x) & \text{if } x < x_L \text{ and } x_L > x_S \\ L & \text{if } x > x_{\max} \end{cases}$$

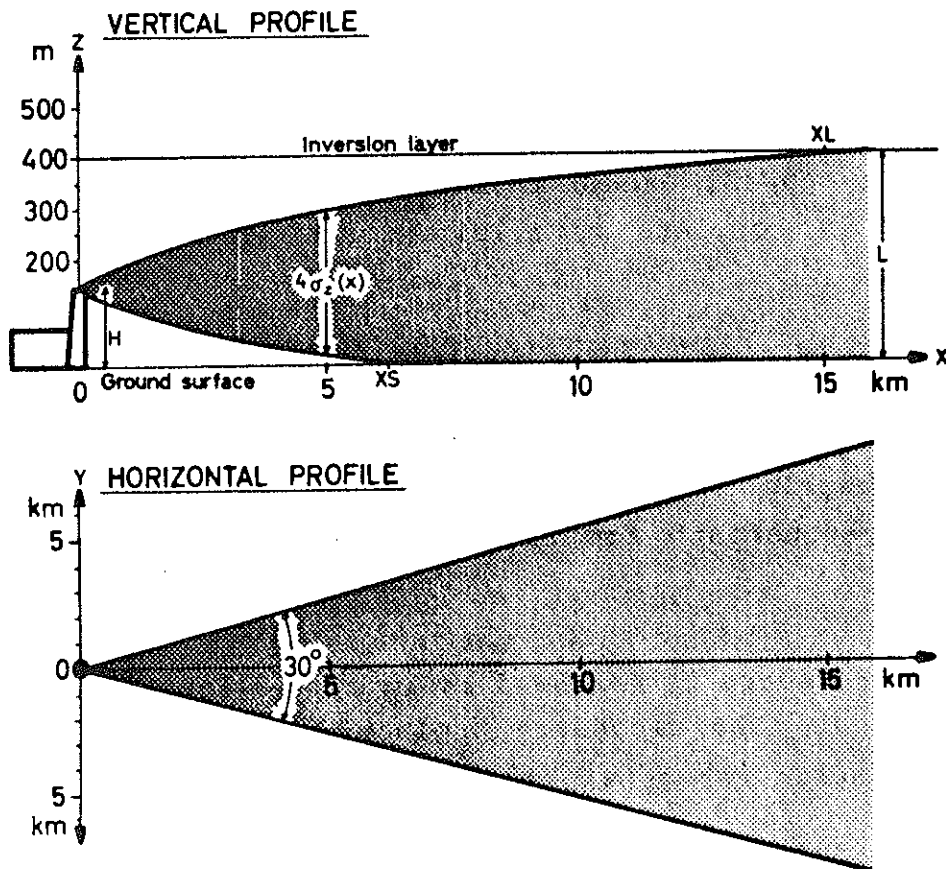


Fig. 3. Illustration of the assumed plume profiles with indication of the distances x_S and x_L .

The meteorological data are long-time averages of frequencies of stability categories, wind speeds, wind directions, and precipitations. The data are drawn from an input file and may, therefore, readily be exchanged with other ones. This would be necessary to do, for instance, if the number of subperiods in a year is changed from the present 2, or whenever the Risoe data are deemed non-appropriate for the actual problem. The structure of the meteorological file is described in more detail under model description.

The compass rose is divided into 12 sectors of 30° as shown in Fig. 4. When the wind is in sector no. 1 it means that the wind is blowing from north towards south.

Whenever the wind direction lies in a certain sector, it is assumed that its direction is exactly in the midline of that sector and that the smoke spreads homogeneously out in the sector.

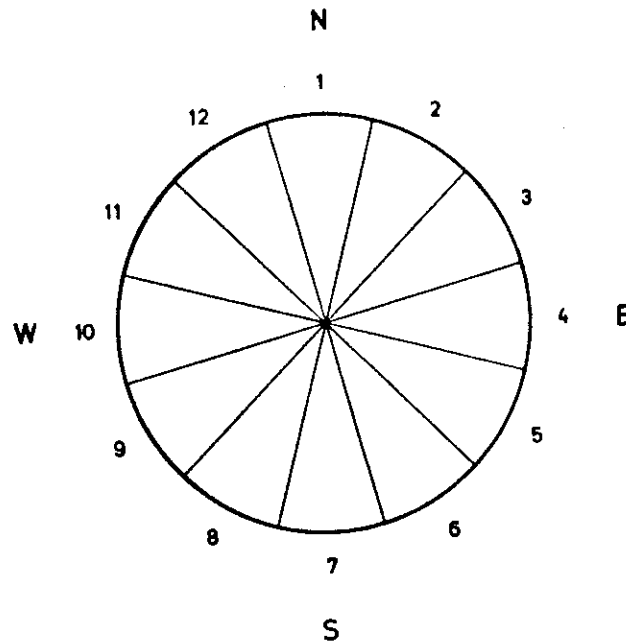


Fig. 4. Windsectors.

In (Højerup 1984) formulae are derived for the concentrations c_1 and c_2 , and the deposition rates d_1 and d_2 of two substances (pollutants) simultaneously, one of which is formed from each other during the transport.

Deposition of a specific pollutant is characterized by the deposition parameter, and the transformation is modelled by ascribing the half life to the emitted pollutant. Deposition velocities may be different for the two chemical forms of the pollutant. This design of the model has been selected since it should be able to model dispersion phenomena associated with SO_2 and NO_x in the atmosphere.

The model is restricted to distances not over 100 km and to time intervals not shorter than one month. Only transformations of the kind where the formation rate of the secondary pollutant is proportional to the concentration of the primary pollutant can be treated.

Pollution from traffic, houses, etc. is usually characterized by being emitted at low heights (< 10 m) and being emitted from a large number of more or less uniformly distributed sources.

For such area sources it is assumed that emission is uniformly distributed throughout the area in which they are situated. All sources are assumed to have the same emission height. This area source is then approximated by N fictitious sources, one situated in the centre of the area and the rest situated equidistant on a circle with centre coinciding with the centre for the area.

Air concentration and deposition of pollutant in a point outside the source area are determined as the sum of contributions from the N fictitious sources.

2.3. Soil chemistry model

The purpose of the theoretical considerations given in the following is the development of a mathematical model which can calculate long term changes of soil chemistry in upper soil layers influenced by acid precipitation or by deposition of polluting materials.

A set of equations are described which in a simplified manner describe the chemical reactions taking place when rain water is percolating through a top soil layer or a succession of soil layers below each other. Each layer is regarded as a completely mixed compartment. Ion exchange reactions as well as the carbon dioxide equilibria and the precipitation or dissolution of chalk or gypsum are taken into account. The result of the model calculation is the time development of the soil pore water composition which then may serve as basis for the calculation of uptake of polluting materials in plants.

The model is an attempt to simulate a very complex system. Many simplifications have been necessary and further refinement may be required before a satisfactory simulation of reality can be made. The model as it stands has been developed for arable soil. The simulation of for example forest soil will probably require extensive modifications.

The soil may be divided into 5 layers. Each layer is treated as a homogeneous compartment containing solid material, soil liquid (water) and air.

The vertical movement of water through the soil layers is described by a simple hydrology model. Each layer is assumed to be able to contain up to a maximum amount of water. Furthermore a minimum amount of water is supposed not to be available for root uptake or evaporation. In the uppermost layer water may be added by rain or irrigation in known quantities. The evaporation is assumed to be known. Water uptake in crops is calculated by the crop model. If the amount of water added to the soil layer by these processes exceeds the amount required to fill the layer to its maximum inventory, the exceeding water is assumed to percolate to the following layer. The layers beneath the uppermost layer are treated in the same way, except that direct evaporation is assumed zero.

All types of soil contain materials which to some degree have ion-exchange properties. It can be various clay minerals, humic material, hydroxides of aluminium, iron, manganese, etc.

Soil ion-exchange can be subdivided into three different types of mechanisms: Cation-exchange due to 1) a permanent, 2) a variable cation-exchange capacity which in the following will be designated CEC_p and CEC_v , respectively, and 3) an anion-exchange capacity designated AEC. The capacities are given in meq exchangeable ions per 100 g of dry soil. Some examples of the reactions involved in the ion-exchange processes are shown schematically in Fig. 5.

2.3.1. The permanent ion-exchange capacity

The permanent ion exchange capacity CEC_p is mainly due to negative charges covering the surfaces and edges of clay particles in the soil. Typical values for CEC_p are 1 to 100 meq/100 g, much dependent on the type and content of clay in the soil.

It has been found that the permanent ion exchange capacity is practically completely saturated by Ca^{++} , Mg^{++} , and Al^{+++} ions. A small amount of H^+ ions will also be bound by the electrostatic forces, but normally in concentrations, which are much lower than for the cations mentioned above. The reason is partly that the concentration of hydrogen ions - even in strongly acid soils (pH 4-5) - normally is considerably lower than the concentrations of other cations in the pore water, and partly that clay particles, at least in thin solutions, in the same way as other strong ion-exchange materials are adsorbing di- and multi-valent cations more strongly than mono-valent ions such as H^+ . The result of the same property is that only a small part of the capacity is normally saturated with Na^+ and K^+ ions. However, K^+ and NH_4^+ are bound somewhat better than Na^+ . This is important since it delays the loss of important fertilizers due to leaching.

ION-EXCHANGE MATERIAL solid phase.		Water phase	
Anion-exchange capacity	$\begin{array}{c} -O \\ \diagup \\ -O \end{array} Al-OH$	$+ SO_4^{--} + 2 H^+$	
AEC	$\begin{array}{c} -O \\ \diagup \\ -O \end{array} Al-SO_4^-$	$H^+ + H_2O$	
Associated with hydrated oxides of Al, Fe and Mn			
<hr/>			
Variable cation-exchange capacity	$\begin{array}{c} -O \\ \diagup \\ -O \end{array} Al-O^-$	$Me^+ + H^+$	
CECV	$\begin{array}{c} -O \\ \diagup \\ -O \end{array} Al-OH$	$+ Me^+$	
Associated with hydrated oxides of Al, Fe and Mn			
or	$-COO^-$	$Me^+ + H^+$	
organic materials	$-COOH$	$+ Me^+$	
<hr/>			
Permanent cation-exchange capacity	-	$Me^+ + H^+$	
CECP	-	$H^+ + Me^+$	
Associated with the permanent electrical charges on surfaces, etc.			
	$Al(OH)_3$	$3 Me^+ + 3 H^+$	
	\rightleftharpoons	$Al^{+++} + 3 Me^+ + 3 H_2O$	

Fig. 5. Schematic presentation of the three types of ion-exchange processes which may occur in connection with solution/solid phase reactions in soil.

A small part of the capacity will also be used for trace materials such as the micro-nutrients Cu^{++} , Zn^{++} , etc. or toxic materials such as Cd^{++} .

The permanent ion-exchange capacity C_p (eq/l(system)) can be written as

$$C_p = J \cdot \rho_j \cdot \text{CEC}_p / (100 \cdot D) \quad (1)$$

where J is soil material volume (l), ρ_j is the density of soil material (kg/l), CEC_p is the permanent ion exchange capacity (meq/100g soil) and D is total volume of the soil system (l). The definition of base saturation is introduced

$$B = 2(\text{CaX} + \text{MgX}) / C_p; \quad 0 \leq B \leq 1 \quad (2)$$

where the suffix X indicates that the ion is adsorbed on the permanent ion exchange material. Base saturation is a measure of the degree the ion-exchange capacity which is covered by ions with strong base properties, in this model expressed by Ca and Mg .

In a model simulating nutrient losses from rainfall acidity (Reuss, 1980) the use of the lime potential ($\text{pH} - 1/2 \text{p}(\text{Ca}+\text{Mg})$) was discussed. The lime potential can be expressed as a function of basesaturation

$$\text{pH} - \frac{1}{2} \text{p}(\text{Ca}+\text{Mg}) = 2.98 + \log \frac{B^3}{(1-B)^2} \quad (3)$$

This function is shown graphically in Fig. 6. It is seen that there is not much variation of the lime potential with B in the interval $0.2 < B < 0.9$ (Brodersen, 1984).

The relation between the adsorbed amounts suffix X of Ca and Mg and the activities Caa and Mga in the solution is given by

$$\frac{\text{CaX}}{\text{MgX}} = \frac{\text{Caa}}{\text{Mga}} \cdot k_{\text{Ca/Mg}} \quad (4)$$

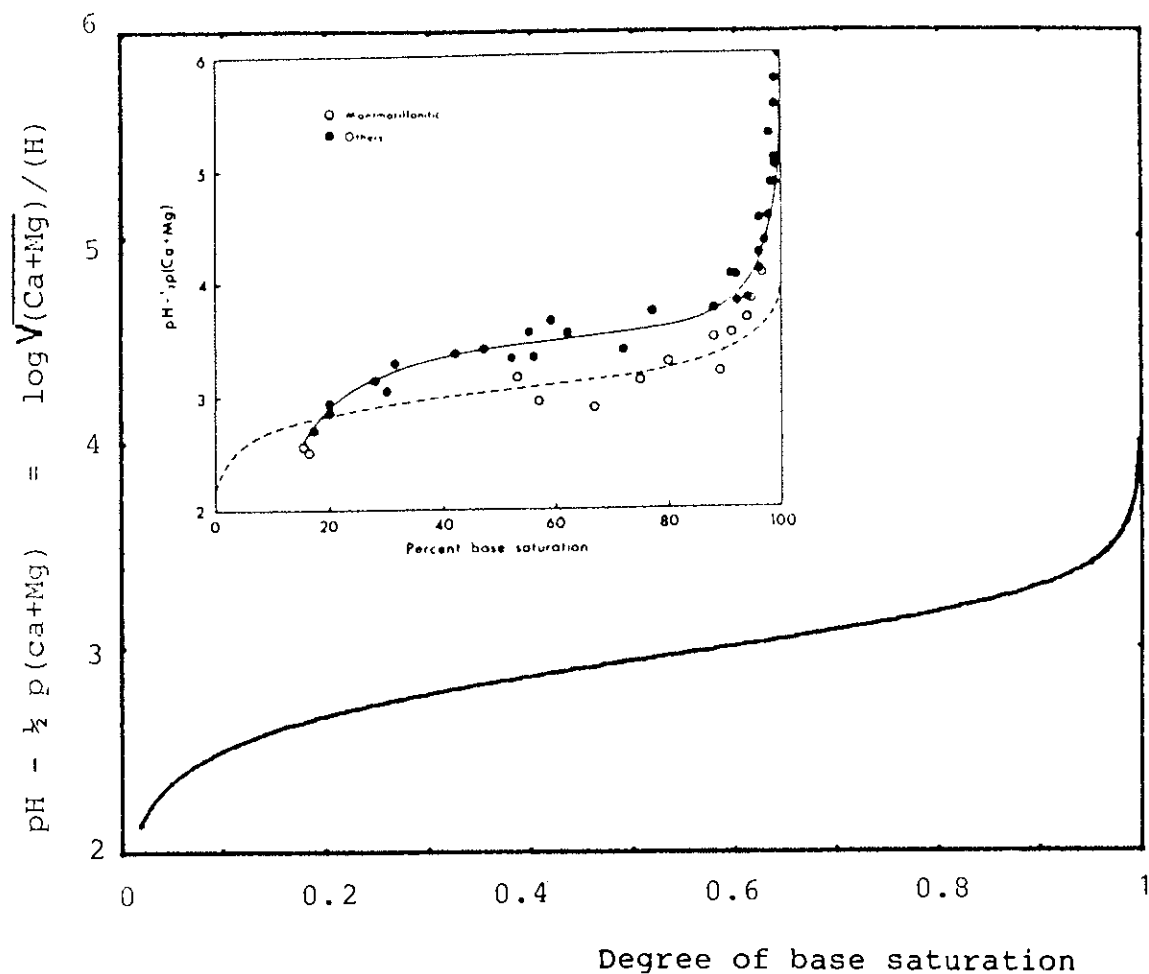


Fig. 6. Lime potential as function of base saturation. Theoretical expression compared with experimental results (Clark and Hill, 1964).

$k_{Ca/Mg}$ is 1.5-5 for kaolinite, 4.4 - 2.2 for illite and 2.7 - 1.7 for montmorillonite depending on the degree of base saturation and the type of clay mineral (Wiklander and Ghosh, 1970). $k_{Ca/Mg} = 3$ is selected as a typical mean value.

Similar relationships based on the law of mass-action describes the relative adsorbance of other ions, i.e. Na^+ , K^+ , NH_4^+ , Cd^{++} , etc. They are supposed only to cover an insignificant part of the total capacity.

2.3.2. Variable ion exchange capacity

The variable ion exchange capacity CEC_v of a soil is due to the presence of materials with ion exchange properties but with the additional property that they are converted to not dissociated components by reaction with hydrogen ions. It can be weak organic acids; phenolic groups in the soil organic material, or precipitated more or less hydrated oxides of Al, Fe or Mn, see Fig. 5.

It is typical for CEC_v that it is changing with changes in pH so that the capacity is zero or small at low pH (The undissociated form) and increasing towards a maximum value CEC_{vmax} with increasing pH. The principle is the same as for synthetic weak ion exchange resins, but it is characteristic for soil materials that the capacity change do not take place at a specific pH value, but more or less continuously over a long pH interval.

A reasonable approximation to the variation of CEC_v (meq/100g soil) to the pH of soil solution is

$$CEC_v = \begin{cases} 0 & \text{for } pH \leq 4 \\ CEC_{vmax} \cdot \left(\frac{pH}{4} - 1 \right) & \text{for } 4 < pH \leq 8 \\ CEC_{vmax} & \text{for } 8 < pH \end{cases}$$

The formula for the variable ion-exchange capacity C_v expressed in eq/l (system) is similar to equation (1):

$$C_v = J \cdot \rho_j \cdot CEC_v / (100 \cdot D) \quad (5)$$

It follows that the presence of a variable ion-exchange capacity in neutral or alkaline soils represents a resistance against pH variation which must be combined with the corresponding adsorption effect of the permanent ion exchanger.

Moreover it is assumed that

$$C_v = 2(CaV + MgV) \quad (6)$$

where the suffix V indicate that the ion is adsorbed on the variable ion exchange material.

The relative distributions between the absorbed ions are given by similar formulas as for the permanent ion exchange sites, equation (4).

2.3.3. Anion exchange

Some soil materials have besides the cation-exchange ability also a certain, normally much lower, anion exchange or adsorption capacity AEC meq/100 g. In most cases the phenomenon is assumed to be due to the presence of hydrated oxides of Al, Fe or Mn, since such materials to some degree will be able to adsorb for example SO_4^{--} on the expense of hydroxyl ions. The resulting oxy-, hydroxy-, sulphate containing Al compound may thereafter be able to contribute to the cation exchange capacity, see Fig. 5.

Conversion to the acidic form requires therefore two hydrogen ions per absorbed SO_4^{--} (1 meq⁺ H^+ per meq SO_4^{--}). At the same time an Al-OH site is consumed, which at least potentially might have contributed to the variable cation exchange capacity. However, the two types of reaction proceed in different pH ranges, so that the same site at least in principle could participate in both processes. Anion exchange is mainly important in acid soils. Formulas describing the phenomenon is

$$\text{SOY} = \text{AC}_{\text{max}} \cdot \text{SO}_4 \cdot f_{\text{ph}} / (k_{1/2} + \text{SO}_4) \quad (7)$$

where

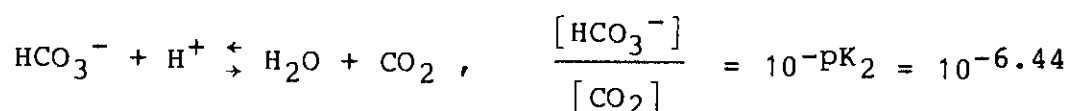
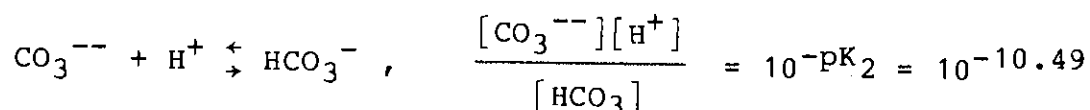
$$\text{AC}_{\text{max}} = J \cdot \rho_j \cdot \text{AEC}_{\text{max}} / (100 \cdot D)$$

$$f_{\text{ph}} = \begin{cases} 0 & \text{for } \text{ph} \geq 8 \\ 2 - \frac{\text{ph}}{4} & \text{for } 8 > \text{ph} > 4 \\ 1 & \text{for } 4 > \text{ph} \end{cases}$$

AEC_{max} is the maximum anion exchange capacity measured in meq/100 g. SOY is the sulphate concentration in the ion exchange material measured in mol/l (system) and SO₄ the sulphate concentration in the soil water. k_{1/2} is the half saturation coefficient.

2.3.4. Chemical equilibria

In addition to the above certain chemical conditions must be satisfied. In soils above pH 5 the HCO₃⁻ ion is an important constituent. The concentration of this ion is controlled by CO₂ pressure and estimated from the following reaction



$$[\text{CO}_2] = c_{\text{CO}_2} - p_{\text{CO}_2} = 0.054 \cdot p_{\text{CO}_2}$$

(at 10°C and solutions with low ionic strength) (Eriksson and Holton, 1974).

This makes the following equations for estimation of CO₃⁻⁻ and HCO₃⁻ concentration;

$$\text{HCO}_3 = [10^{(-6.44-1.27+\log p_{\text{CO}_2}+\text{pH})}]/G1 \quad (8)$$

and

$$\text{CO}_3 = [10^{(-10.49+\log \text{HCO}_3+\text{pH})}]/G2 \quad (9)$$

pCO₂ is the partial pressure of CO₂ in the root zone. G1 and G2 are the activity coefficients for ions with one or two charges respectively. The hydrogen ions used in the two reactions are estimated as the difference in HCO₃⁻ concentrations and in CO₃⁻⁻ concentration within a timestep.

The system takes precipitation or dissolution of chalk (CaCO_3) and gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$) into account. E.g. when the concentration of calcium is higher than corresponding to the solubility product for CaCO_3

$$[\text{Ca}^{++}] > 10^{-8.15}/[\text{CO}_3^{--}] \quad (10)$$

precipitation of calcium carbonate is taking place. Otherwise chalk added at the surface is going into solution under hydrogen ion consumption.

2.3.5. Mass balances

For all ions mass balance equations for estimation of the concentration are set up which include the following elements:

$$I_t = (I_{to} \cdot M_{to} + I_{in} - I_{pl} + I_{CP} + I_{CV} - I_W) / (M + P) \quad (11)$$

I_t is the concentration (mol/l) of dissolved ions in the soil solution at the time t . I_{to} is the concentration at time to and M_{to} the watercontent in the soil layer at time to . I_{in} is the amount of ions added from the outside with rainwater, fertilizer etc., while I_{pl} is the amount taken up by plants. I_{CP} and I_{CV} stands for the change in contents on the ion exchange materials at the permanent and variable ion exchanger respectively. For sulphate input from the anion exchanger is incorporated instead of I_{CP} and I_{CV} . I_W is the amount of ions precipitated or dissolved as lime or gypsum. $(M+P)$ is the amount of water in the soil layer after summation of all water input in the timestep. P is the amount of water percolating to the soil layer below.

The electroneutrality of the system is maintained at each time steps. All together a total of 18 equations are solved simultaneously for each compartment and time step to obtain $[\text{H}^+]$ and other concentrations.

The system is further complicated by the need to use activities instead of concentrations in the equations based on the law of mass-action, etc. The activity coefficients are estimated accord-

ing to the general Debye Hückel theory (Baes and Mesmer, 1976) by the simplified expression

$$\log G_i = - \frac{z^2 \cdot 0.511 \cdot \sqrt{I}}{1 + \sqrt{I}} \quad (12)$$

where z is the charge and the ionic strength I is given by:

$$I = \sum (z_i^2 \cdot [i]) \quad (13)$$

The equations are solved using interactive procedures.

As an appendix the total concentration of dissolved Al in equilibrium with $\text{Al}(\text{OH})_3$ (as gibbsite) is obtained by summation of the contributions from Al^{+++} , $\text{Al}(\text{OH})_2^+$, $\text{Al}(\text{OH})_3$, and $\text{Al}(\text{OH})_4^-$ estimated as:

$$\begin{aligned} \log(\text{Al}^{+++}) &= 8.5 - 3\text{pH} \\ \log(\text{Al}(\text{OH})_4^-) &= -14.5 + \text{pH} \\ \log(\text{Al}(\text{OH})_3) &= -6.5 \\ \log(\text{Al}(\text{OH})_2^+) &= -0.8 - \text{pH} \end{aligned}$$

This simple treatment overestimates the concentration of Al^{+++} in acid soil.

2.4. Crop model

Crops growing on a soil will influence the soil chemistry by uptake of water, nutrients, micro nutrients and trace metals. Plants also form part of the pathway for certain elements, e.g. heavy metals, to animals and man.

The crop model included in the ECCES system has been set up to model these effects (Mortensen, 1984). The intention is to calculate the chemical effects on the soil upon which the plant grows and the amount of trace element taken up by the plant.

The basis for the plant model is a table which has the above ground biomass production and the associated water uptake from the soil tabulated on a monthly basis for the growing season. In the same table evaporation from soil surface is given. These values are used for the hydrology model in the soil chemistry model.

The uptake of nutrients and trace elements via the root system is assumed to be proportional to the uptake of water multiplied by concentration of the ions in the soil water as obtained from the soil chemistry model. Ion uptake ION_{opt} ($\text{mol} \cdot \text{m}^{-2} \cdot \text{month}^{-1}$) is described as

$$ION_{opt} = W_{up} \cdot C_{ion} \cdot K_{up} \quad (14)$$

where W_{up} is the water uptake ($\text{l} \cdot \text{m}^{-2} \cdot \text{month}^{-1}$), C_{ion} is the ion concentration in interstitial water ($\text{mol} \cdot \text{l}^{-1}$), and K_{up} (no unit) is the uptake coefficient dependent on the crop type and ion.

Introduction of the uptake coefficient is for calibration purposes and shall be looked upon as a selectivity coefficient, i.e.

$K_{up} > 1$ for active ion uptake

$K_{up} = 1$ for passive ion uptake

$K_{up} < 1$ for discrimination against the ion uptake

The response to uptake of ions in plant roots is excretion of either H^+ or OH^- ions (Wiklander, 1977, and Reuss, 1977) to maintain ion neutrality in soil and plant tissue. Release of H^+ is a consequence of excess uptake of positive ions and results in acidification while over-uptake of negative ions results in release of OH^- and a tendency to alkaline reaction in the soil water (Fig. 7).

It is assumed that water uptake from a certain soil compartment is proportional to the root density estimated as cm living root biomass pr. cm^3 soil.

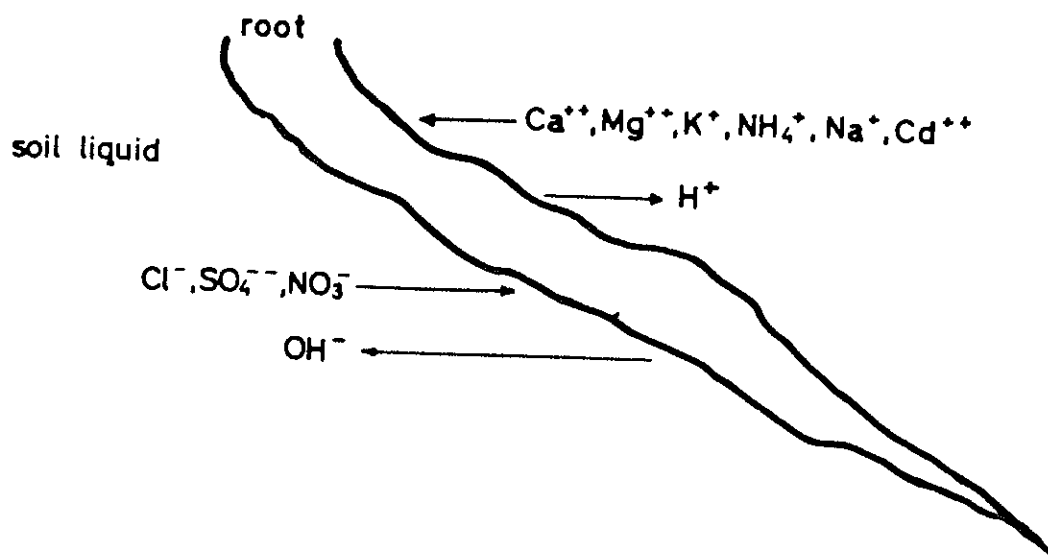


Fig. 7. Uptake of nutrients and pollutants from soil liquid, and release of H^+ and OH^- .

The root distribution coefficients (RDC) describes the fraction of root per centimeter soil, in a certain soil layer. Summation of all RDC down through a root zone gives a total of one.

The fraction of root (F_{roi}) in soil layer (i) with the upper border (I_i) and lower border (I_j) (Fig 8) is calculated as

$$F_{roi} = \frac{I_j}{\sum_{I_i} \text{RDC}}$$

If the total water uptake per month from a soil is W_{tup} then the uptake of water from soil compartment (i) ($\text{mm} \cdot \text{month}^{-1}$) is

$$W_{upi} = W_{tup} \cdot F_{roi} \quad (15)$$

If the water uptake is greater than the available water in a certain soil compartment the deficit water is supposed to be taken up from the next lower compartment.

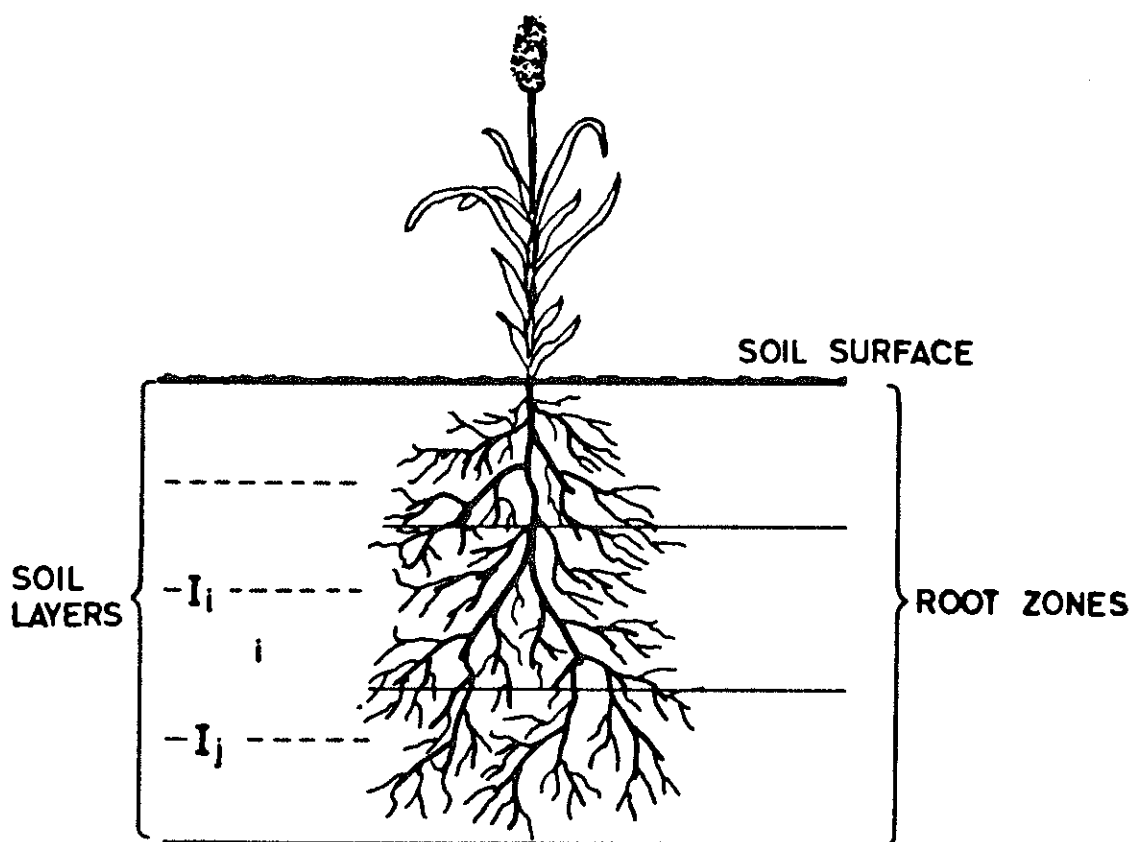


Fig. 8. Soil layers and root distribution. I_i is the upper surface of lay i , I_j is the lower surface.

Some of the ions depositing from the air are directly intercepted on the vegetation surface, which in this way filtrate a fraction of the depositing materials. The remaining fraction penetrates the herbage and deposit on the soil beneath it. The degree of the intercepted material (aerosols and gasses) is dependent on many physical and biological conditions which are very difficult to model mathematically.

In the model the herbage is represented as a single homogenous filter. Chamberlain (1970) introduced the concept of a simple filtration model to describe that fraction of depositing aerosols which is intercepted by the herbage upon which it impinges.

This description of direct interception of air pollutants on the vegetation UP_{air} ($\text{mol} \cdot \text{m}^{-2} \cdot \text{month}$) are used in the present model

$$UP_{air} = F \cdot DEP \quad (16)$$

$$F = 1 - \exp(-My \cdot W)$$

where F is the fraction intercepted on the vegetation, DEP is the total deposition of the pollutant, calculated from the air pollution model ($\text{mol} \cdot \text{m}^{-2} \cdot \text{month}^{-1}$), My ($\text{m}^2 \cdot \text{kg}^{-1}$) is the filtration parameter with values around 2.3-3.3 (Chamberlain, 1970), W is the herbage areal density ($\text{dry weight} \cdot \text{m}^{-2}$)

Because of rain, wind and fall off from dying back there will be a flow of intercepted material to the soil surface. This wash off rate R_{wof} ($\text{mol} \cdot \text{m}^{-2} \cdot \text{month}^{-1}$) is described in a simple way

$$R_{wof} = C_{wof} \cdot C_{out} \quad (17)$$

where C_{wof} is the wash of constant ($0.037-0.054 \text{ day}^{-1}$) (Chamberlain, 1970), and C_{out} ($\text{mol} \cdot \text{m}^{-2}$) is the content on the surface of intercepted ions. The wash of constant must be adjusted to obtain known concentration levels described in the literature.

2.5. Model structure

The program is written in FORTRAN-77 and it is implemented on a Burroughs B7800 computer at Risø National Laboratory. The implementation is done in single-precision which on a Burroughs computer means about 11 significant digits. Some of the calculations, especially in the model for the soil chemistry, are rather sensitive to small changes, so tolerances of magnitude 10^{-8} are required. Therefore, the program cannot without special care be moved to other computers with less precision.

The program is at the present level divided into three main parts:

1. Reading and checking of input and definition of scenario.
2. Calculation of pollutant dispersion from sources to recipient areas.
3. Calculation of conversions in soil and absorption in crops.

The intention is to make the program as general as practically possible, but still rather easy to use. It is always a problem where to draw the line between generality and simplicity, because they pull in opposite directions, but here it is circumvented with a system of data-base-like files from which the data to the actual simulation are fetched.

The general input is read from the normal FORTRAN input file. Each input item is printed out and tested for allowability and sometimes also for probability.

The program can either be started from new or restarted from a previous run. The final dump at the end could either be done at the end of the simulation or after a specified CPU-time.

The model is explicitly programmed, which means that calculation procedure is as follows (Fig. 9).

- A. Calculate the deposition velocity with the dispersion model for one large time step.
- B. Take one (smaller) time step with the soil and crop uptake model.

The subroutine HYDRO calculates the changes in the pore water content in the different soil layers and the water uptake by the crops during the time step. The supplies to the upper soil layer are rain and irrigation water and to the deeper layers it is percolation from the above layer. Removals are by evaporation, uptake in crops and percolation to the underlying layer.

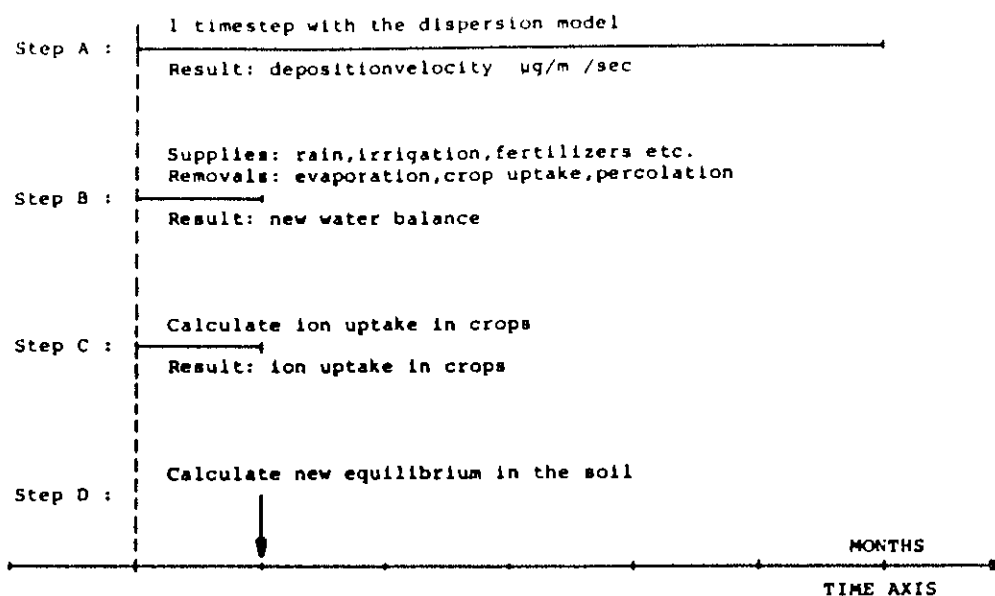


Fig. 9. The calculation progress with different timestep sizes and the four major calculation steps.

- C. In the subroutine PLANT the ion (pollutant) uptake to the crops is calculated. The ion uptake is based on the ion concentration in the soil before the time step and the water amount calculated in HYDRO. This causes a change in the water and ion contents in the soil as do the contributions from rain, irrigation, fertilizers and evaporation (but not percolation!). This is the explicit formulation; there is no iteration between crop uptake and the soil concentrations during the time step.
- D. With all the changes in water and ion contents known a new equilibrium situation in the upper layer of the soil is calculated. These new ion concentrations are then used in the possible percolation to the next layer, where a new equilibrium in SOILCH is calculated and so on.
- E. When all the soil chemistry iterations have converged take a new time step.

The output from the new calculations is partly the contents of pollutants in the harvested crops from a whole area and partly the changes in the soil of pH and ions previously described.

The uptake in crops are accumulated to the time for harvest and are then saved for a joint print out of all crops. (They are not all harvested at the same time of year).

In the soil model (subroutine SOILCH) there are three iterations inside one another. The outer one is an iteration in the ion strength and it is no problem, but the inner iterations in pH and base saturation are rather difficult, because they often diverge or at best converge very slowly with ordinary iterations. The difficulties have been handled by combining different techniques depending on the range of the solutions. The techniques include direct iterations, NewtonRaphson iterations, extrapolation with relaxation and the bisection method. Which method to be used is purely empirical, but the bisection method is used as a last resort, when the other methods fail to converge in a limited number of iterations.

The time step length in the soil and crop uptake model can be chosen by the user, but there is one restriction. The step size should fit with the the step size used in the dispersion calculations, which means that there should be an integer number of steps for each step with the dispersion model.

Seven data files contain the basic data for the ECCES-program. Each file is organized in a database-like structure, where each major item consists of a fixed number of records. For each file the number of records for each item is given.

Meteorological data are on a file METDATA. It contains statistical data, appropriate for the geographical area under consideration, for 12 wind directions (30° sectors), 7 stability categories (the Pasquill categories) and 5 wind velocity groups, rainfall and evaporation data.

The data file for areas (DBAREAS), plants (DBPLANTS), and cities (DBCITIES) contain data for positions, source strength with more. Specially for areas and cities the data files contain areas for soil types and for crops in that area or city, respectively.

The data file for crops (DBCROPS) contains biomasses and water uptake rates for the crops.

The data file for soil types (DBSOIL) contains specific parameters for that pollutant such as mole weight, valency, deposition velocities. Furthermore it contains start concentrations for the pollutant in each soil type and uptake coefficients for each crop.

All these data files are permanently stored and the data structure is illustrated in fig. 10.

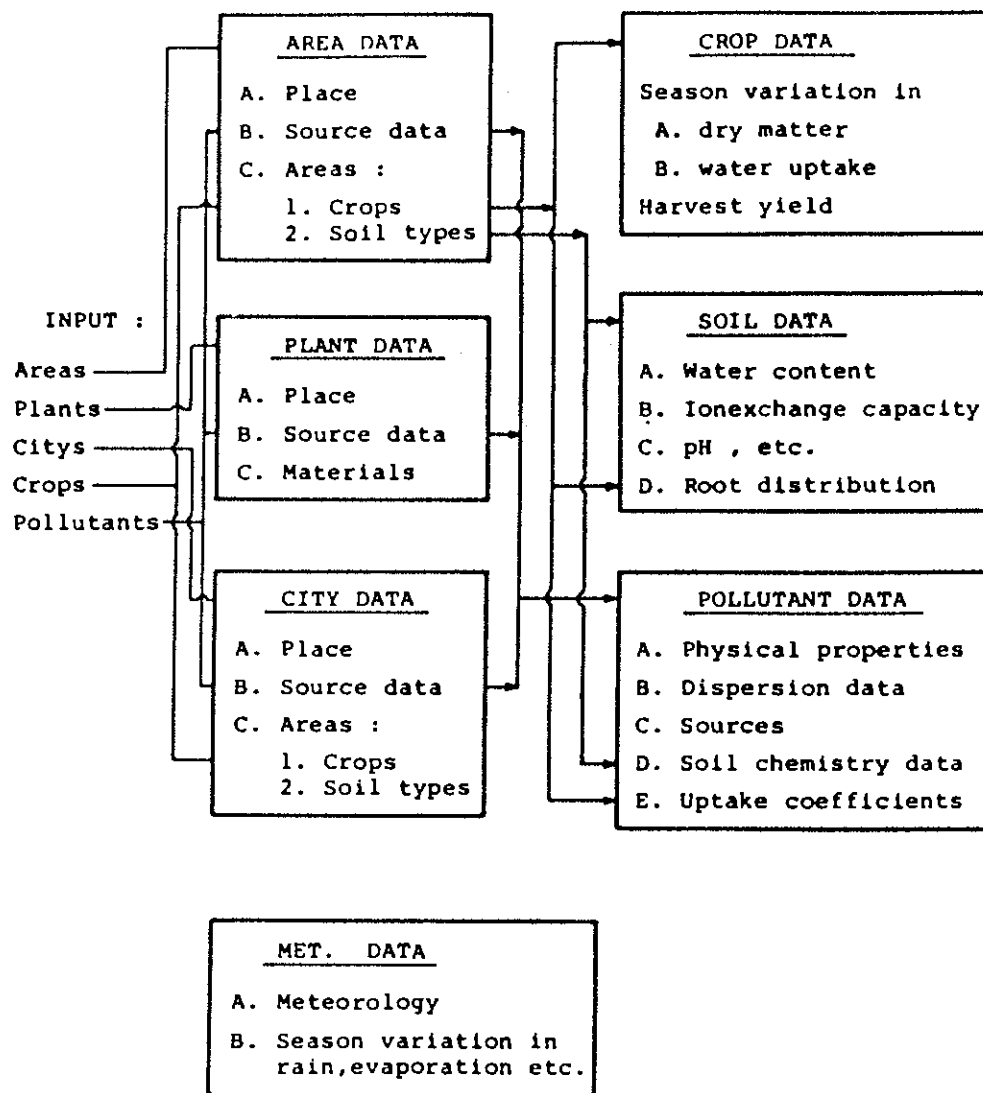


Fig. 10. Data structure. Areas, plants, cities, crops, and pollutants are selected from input.

There will be data which may logically belong to more than one data file. E.g. characterization of uptake of a certain pollutant in a certain plant may either be considered a property of the pollutant or the plant. Such data is stored in order to give the largest flexibility when the data is used.

As the model is used for new scenarios the data bank shall expand. By keeping a catalogue which shows the identification numbers of pollutants, soil types, subareas, etc. one may go back and reuse already collected data for new scenarios without having to set up large amounts of input data.

If f.ex. one has run a scenario with Cd as pollutant one may run the same scenario with Hg as pollutant simply by changing the identification number of the pollutant, if provided data for Hg is present in the data bank.

3. A SCENARIO EXAMPLE

As an example of the capacity of the model a scenario with Roskilde Amt as influenced by seven power plants on the island of Zealand, has been set up, see Fig. 1. Two different crops: winter cereals and grass is simulated in Roskilde Amt. This scenario is simulated first for 20 years with the power plants at full power and then further for 10 years with all power plants at zero power (Christensen et al., 1985).

The print result of the dispersion calculation for sulphur SO_2 (plant product) and SO_4^{--} (daughter product) is shown in Fig. 11. This print shows the source strength for all the power plants, the simulated average air concentration in $\mu\text{g}/\text{m}^3$ and the amount deposit in the area for both products. The results are only for illustration purposes.

All curves in the following are based on 12 time steps per year.

YEAR = 1984 'SUBPERIOD' = 1

RESULT OF DISPERSION CALCULATION FOR POLLUTANT NO. 2 SULPHATE

POLLUTION TO AREA NO. 11113000 ROSKILDE ANT

FROM :	SOURCE STRENGTH KG/SEC	PARENT PRODUCT IN AIR MICROG/M3	DEPOSITION G/M2/YEAR	DAUGHTER PRODUCT IN AIR MICROG/M3	DEPOSITION G/M2/YEAR
PLANT NO. 11114011 ASVTOT (180 M)	1.40E+00	1.19E+00	3.25E-01	1.46E-01	1.17E-02
PLANT NO. 11111011 AMVTOT (150 M)	2.70E-01	2.34E+01	6.34E-02	2.90E-02	2.30E-03
PLANT NO. 11112011 KYVTOT (100 M)	8.60E-01	1.12E+00	3.03E-01	1.30E-01	1.02E-02
PLANT NO. 11115011 HAVTOT (60 M)	1.40E-01	8.99E-02	2.41E-02	1.28E-02	9.76E-04
PLANT NO. 11114021 STVTOT (130 M)	4.30E-01	3.80E-01	1.02E-01	5.04E-02	3.85E-03
PLANT NO. 11111012 SHVTOT (100 M)	1.80E-01	1.81E-01	4.85E-02	2.59E-02	1.95E-03
PLANT NO. 11111013 HCVTOT (88 M)	3.10E-01	3.54E-01	9.50E-02	4.92E-02	3.73E-03
PLANTS		3.54E+00	9.61E-01	4.43E-01	3.47E-02
CITIES		0.00E+00	0.00E+00	0.00E+00	0.00E+00
AREA NO. 11113000 RSKLD. (10 M)	8.80E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
AREAS		0.00E+00	0.00E+00	0.00E+00	0.00E+00
TOTAL TO THIS AREA		3.54E+00	9.61E-01	4.43E-01	3.47E-02

Fig. 11. Example of print from the dispersion model.

Soil chemistry and crop uptake calculations have also been made for a 30 year period. The print results are shown in the output example in Fig. 12, which shows the ion concentrations in the crops together with the total quantity of the ions removed from the area that year. The soil chemistry status of the different soils is also given in the print output, in this example the pH of the six soils involved are shown.

Examples of plot curves are shown in Figs. 13 - 15. Fig. 13 shows the content of sulphate in the harvest of the two crops. A characteristic drop in the uptake is seen when the power plants are shut down.

Fig. 14 shows the corresponding curves for cadmium. The cadmium concentration is steadily increasing mainly due to input from fertilizers. When the power plants are shut down the curves shift due to an increase in pH in the soil. The curves are less steep after the plant shut down and the resulting decrease in cadmium supply. Finally Fig. 15 shows the pH-variation in the upper soil layer in the soil (sandy clay) when winter cereals are growing upon it. There is a rather large yearly variation, mainly due to the supply of fertilizers but also due to the growing crops. When the power plants are shut down pH raises about 0.06 units.

UPTAKE IN CROPS IN YEAR : 1995 FOR AREA : 11113000 ROSKILDE AMT

		CONCENTRATIONS IN MICROGR./KG	
POLLUTANT NO.	NAME	W.CER.	GRASS
2	SULPHATE	1.70E+06	1.38E+06
9	NITRATE	4.37E+06	2.68E+06
14	CADMIUM	5.02E+01	3.23E+01
3	CALCIUM	4.40E+06	2.51E+06
5	POTASSIUM	2.16E+06	1.41E+06
6	MAGNESIUM	3.08E+05	1.93E+05
7	SODIUM	1.17E+06	8.66E+05
8	AMMONIUM	3.62E+06	2.33E+06
HARVEST IN KG/M2		1.33E+00	2.70E+00
CROP AREA IN KM2		1.23E+02	3.84E+01

		QUANTITIES IN CROPS IN T/YEAR	
POLLUTANT NO.	NAME	W.CER.	GRASS
2	SULPHATE	2.78E+02	1.43E+02
9	NITRATE	7.15E+02	2.79E+02
14	CADMIUM	8.21E-03	3.35E-03
3	CALCIUM	7.20E+02	2.60E+02
5	POTASSIUM	3.54E+02	1.46E+02
6	MAGNESIUM	5.04E+01	2.00E+01
7	SODIUM	1.91E+02	8.98E+01
8	AMMONIUM	5.92E+02	2.42E+02
HARVEST IN T		1.64E+05	1.04E+05

		ACIDITY AT TIME : JANUARY 1996 PH IN THE UPPER SOIL LAYER	
SOIL NO.	NAME	W.CER.	GRASS
100	COARSE-FINE	5.21	5.14
200	CLAYEY SAND	5.29	5.16
300	SANDY CLAY	5.35	5.45
400	CLAY	5.45	5.72
500	HEAVY CLAY	5.61	5.81
600	ORGANIC SOIL	5.63	5.82

Fig. 12. Example of print from the crop uptake model.

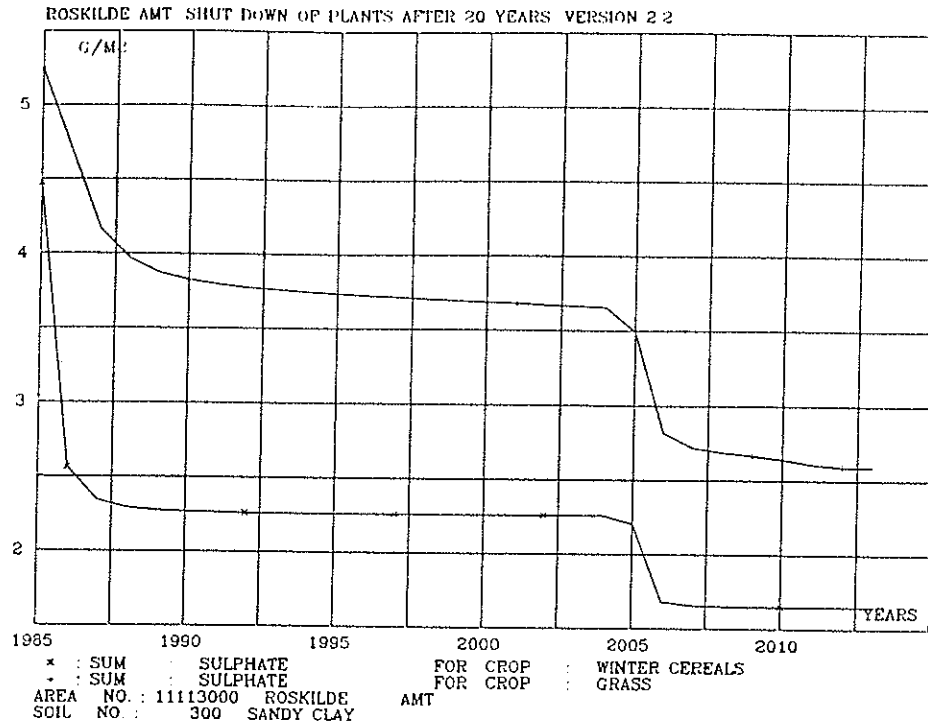


Fig. 13. Uptake of sulphate in the harvest of winter cereals and grass in Roskilde during a 30 year period. The marks on the curves are for identification only.

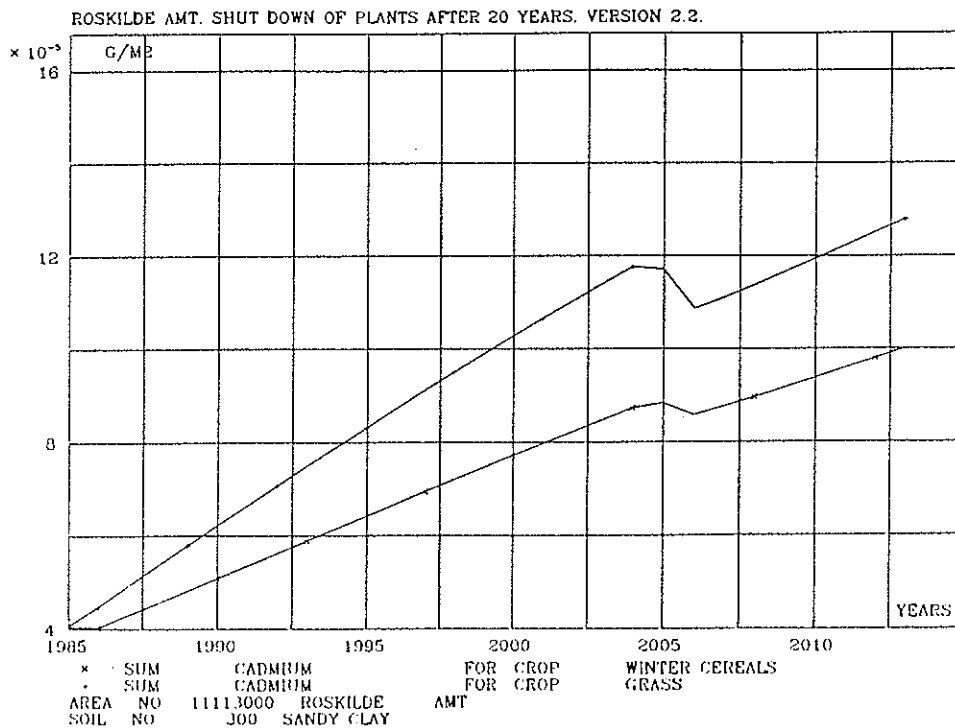


Fig. 14. Uptake of cadmium in the harvest of winter cereals and grass in Roskilde during a 30 year period.

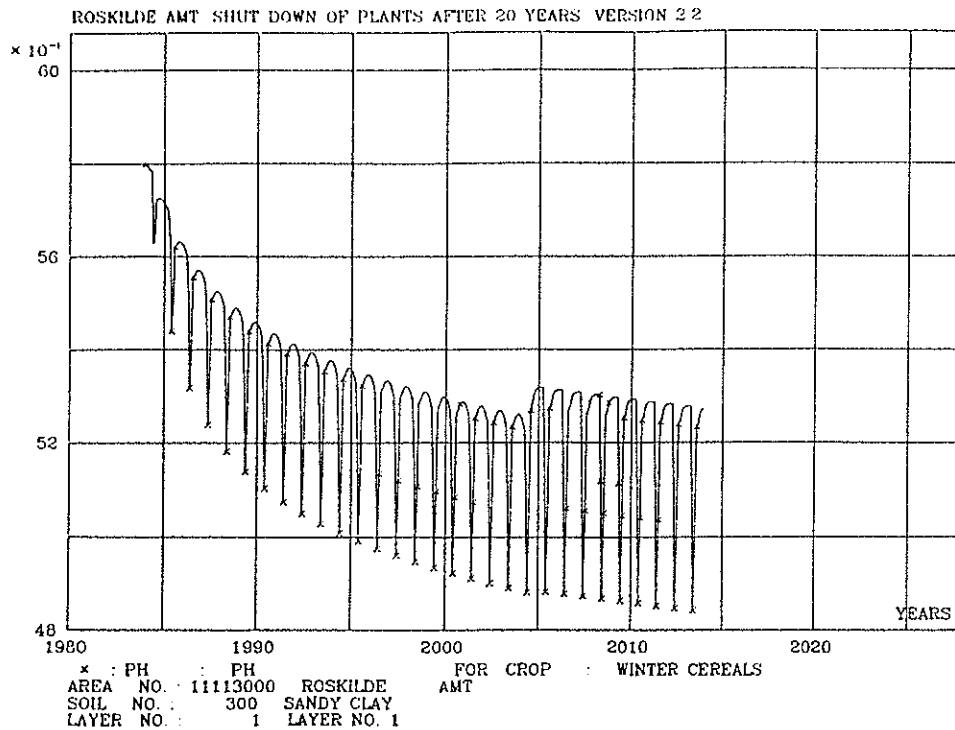


Fig. 15. The variation in pH in the upper layer of the soil type, sandy clay when winter cereals are growing upon it.

4. SENSITIVITY TESTS

Illustration of the capabilities of the program and the sensitivity of some important parameter is done using a four layer test soil. For simplification all the soil layers are given the same soil parameters and start concentrations which makes it easier to compare the time dependent development of pH and ion concentrations down through the soil layers. Most test calculations are run without crops but one calculation with winter cereals growing upon the soil is shown. All results shall be regarded as preliminary because most parameters are only estimates.

Constants used for this calculation are shown in Fig. 16. A permanent ion-exchange capacity (CEC_p) of 10 meq/100 g and a

variable ion exchange capacity (CEC_{vmax}) of 1 meq/100 g are used to describe a sandy-clay soil.

A low anion-exchange capacity for sulphate with maximum capacity of 0.007 (meq/100 g) is assumed.

Layer no.	I	II	III	IV
Soil depth (mm)	200	300	500	1000
Solid content (mm)	120	180	300	600
Max. water (mm)	60	90	150	300
Min. water (mm)	20	30	50	100
Density (kg/l)	2.65	2.65	2.65	2.65
Max.Cap.SO ₄ (meq/100g)	0.007	0.007	0.007	0.007
Halfsat.SO ₄ (mol/l)	0.002	0.002	0.002	0.002
CEC_{vmax} (meq/100g)	1	1	1	1
CEC_p (meq/100g)	10	10	10	10
CO ₂ partial (atm)	0.003	0.003	0.003	0.003
Start water (mm)	60	90	150	300
Start pH	7.0	7.0	7.0	7.0

Fig. 16. Constants used as basis for test calculations.

Adsorption of ions to clay particles relative to cadmium are shown in Fig 17. Ca^{++} is bound somewhat stronger to clay particles than Mg^+ , while K^+ and Na^+ is bound stronger than NH_4^+ .

$K_{Ca/Mg}$	3.0
$K_{K/Ca}$	0.22
$K_{Na/Ca}$	0.22
$K_{NH/Ca}$	0.17
$K_{Cd/Ca}$	0.44

Fig. 17. Adsorption constants.

The rain input (mm) from January to December in this simulation is from Lund and Dorph-Petersen (1971).

Rainfall chemistry used in the simulation is from (Mortensen, 1986) with a proton concentration that makes the pH in rain 4.9.

Start concentrations for all adsorbed ions involved are calculated in the beginning of the program when dissolved concentrations are known.

Permanent adsorbed SO_4^{--} is sulphate adsorbed to the defined anion exchanger of the soil.

Fig. 18 and 19 shows the development of pH in the above defined test soil during 20 years without and with crops. pH in the upper soil layer decreases most rapidly because of the acid rainfall while the effect is delayed down through the soil layers. pH of the soil goes towards 4.9, which is pH of the rain.

Fig. 19 shows the calculated pH in the same soil grown with winter cereals. A yearly variation as a consequence of root uptake of ions is seen. The small peak on the top of every curve are related to the input of fertilizer which influence the ion strength of the soil water creating a small increase in pH. The steep drop especially in the two uppermost soil layers is a consequence of protons released from the crop roots as a response to uptake of more cations than anions. This creates an acidifying reaction in the soil. During wintertime pH increases until fertilizer is supplied again and crops are grown next spring. Soil layer 4 is unaffected by the roots because these mostly grow in the upper soil layers. All the upper soil layers develop a pH about 5 during the winter declining to about 4.6 in the summer. In the test soil without crops (Fig. 18) pH is greater than 5.7 for all soil layers after 20 years.

The ECCES-computer model was also run with a very acid H_2SO_4 -rain with pH = 2, to show the soil pH development as a function of time under such extreme circumstances (Fig. 20).

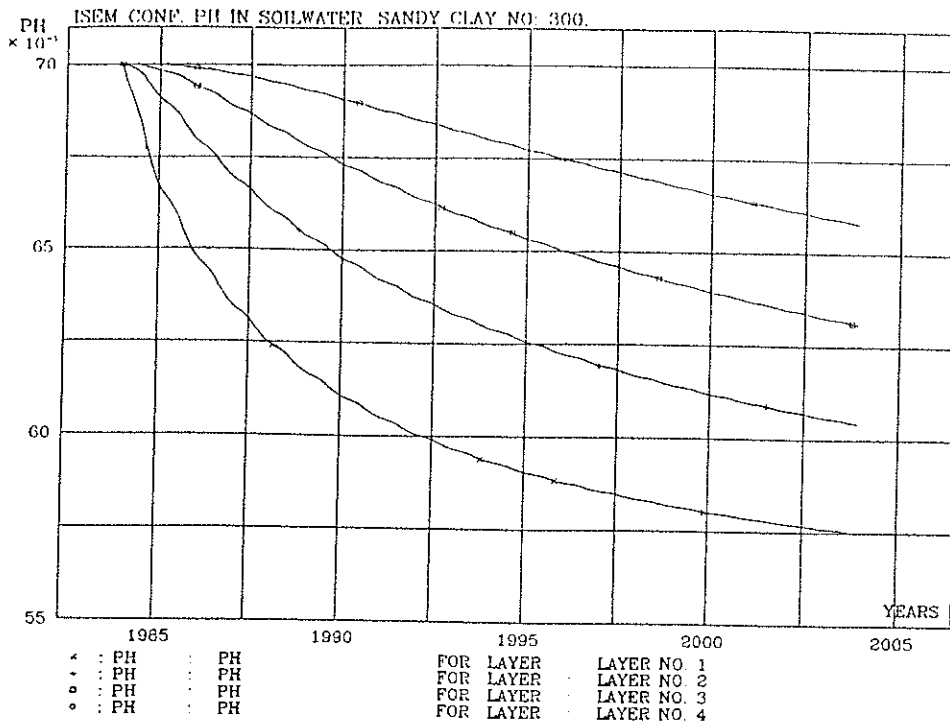


Fig. 18. pH in a sandy clay soil without crops.

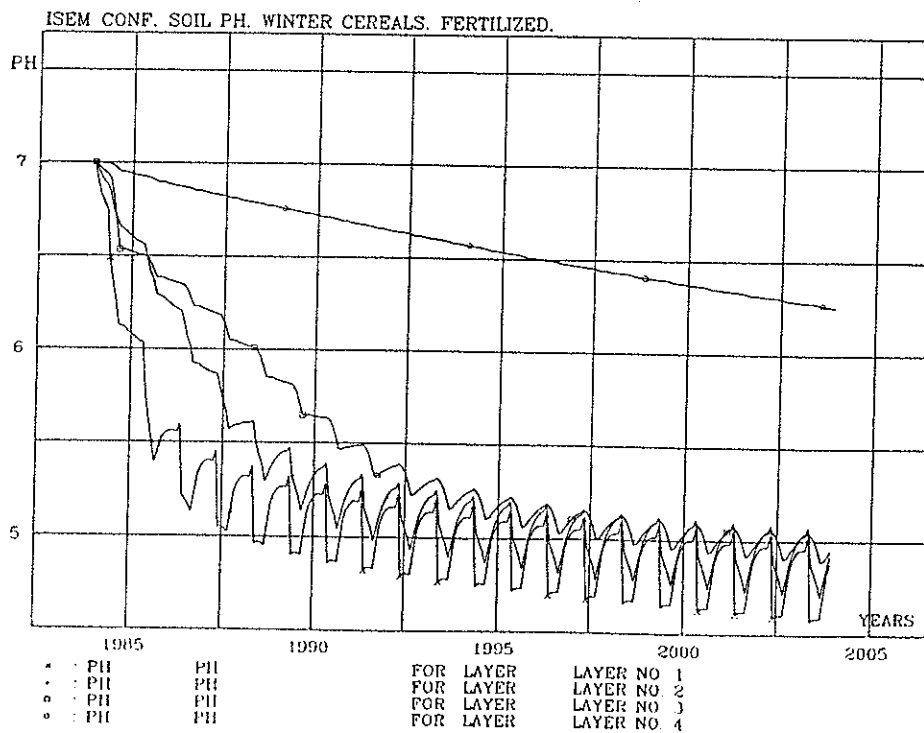


Fig. 19. pH in a sandy clay soil grown with winter cereals.

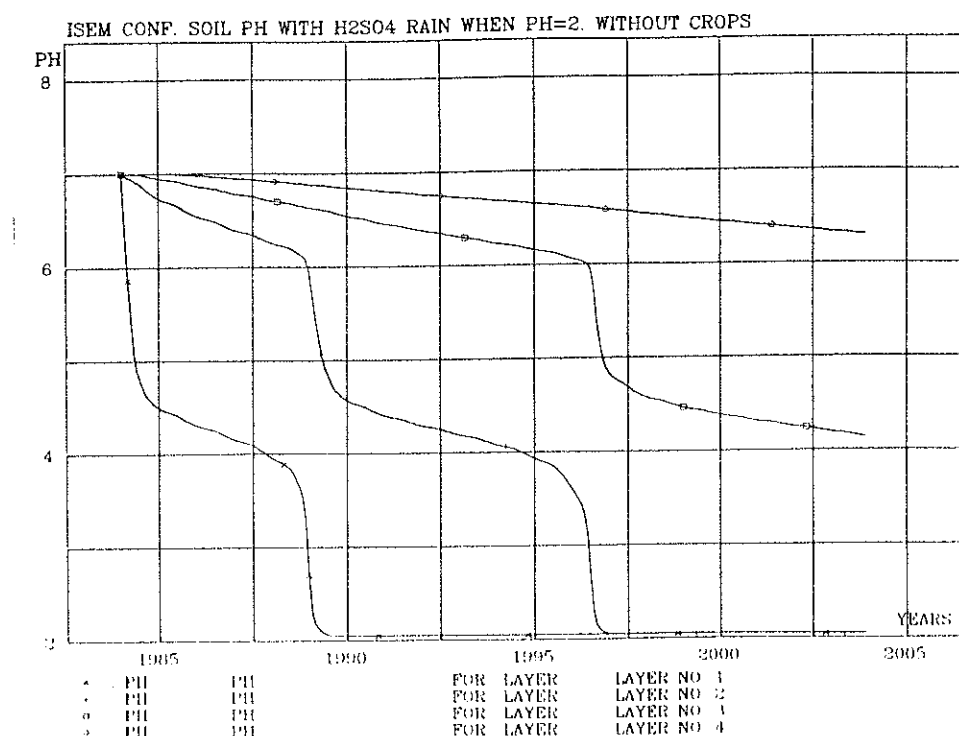


Fig. 20. pH development in a sandy clay soil with a pH = 2 in a H₂SO₄ rain.

This figure shows increasing acidification of all soil layers most pronounced in the upper soil layer with a clear time-lag down through the soil. In the two upper soil layers all the buffer capacity are used up during the simulation. After a very steep drop a plateau is reached in soil layer 1 and 2 for pH = 4.5-3.8. This plateau is primarily a function of the permanent ion exchange capacity.

Fig. 21 shows pH development in the upper soil layer when $CEC_p = 10$ meq/100g and CEC_v range from 0.1 to 10 meq/100g. From the figure it is clear that CEC_v very much influence the buffer capacity of the soil in this pH range. A low value CEC_v (0.1) brings pH down to about 5.6 in the upper soil layer, while a high value (10) create such a strong buffer effect that pH only drops to 6.5 in the upper soil layer during the 20 years.

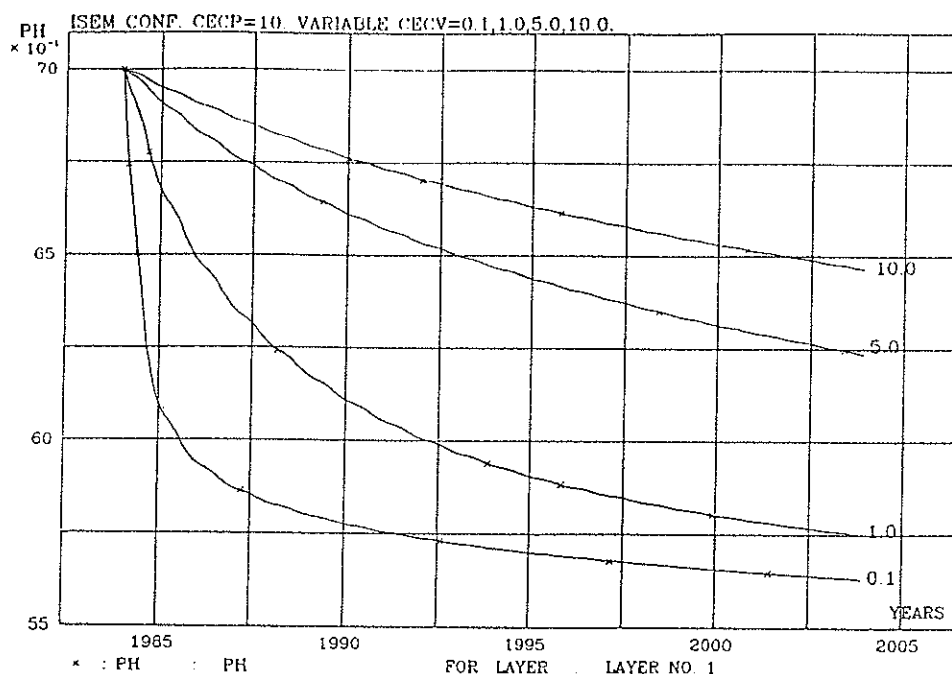


Fig. 21. pH development in a test soil when $CEC_p = 10$ meq/100g and variable CEC_v .

Fig. 22 shows pH development in the soil when CEC_p changes from 1 to 30 meq/100g and $CEC_v = 1$ meq/100g is fixed. CEC_p does not affect the buffer capacity as strongly as CEC_v in this pH interval. Nevertheless CEC_p influences the extension of the plateau shown in Fig. 20 when pH is 3.8 - 4.5. Soils with low $CEC_p = 1$ meq/100 g (very sandy soil) result in a pH of about 5.7 after 20 years, while a very clayey soil ($CEC_p = 30$ meq/100g) results in a pH of 5.8 after 20 years of simulation.

These tests shows that pH in this model is very sensitive to changes in the variable cation exchange capacity in the pH interval from 5.6 to 7. Determination of this parameter is important for the description of pH in this interval.

pCO_2 was also found to be an important parameter for estimating pH when leaching experiments with soil, with experimentally found $CEC_p = 9$ meq/100g and $CEC_v = 9$ meq/100g, was simulated. In the experiment pCO_2 was not controlled but successively change of this parameter resulted in good pH simulations when $pCO_2 \sim 0.002$. A realistic description of pCO_2 in the soil solution is therefore important.

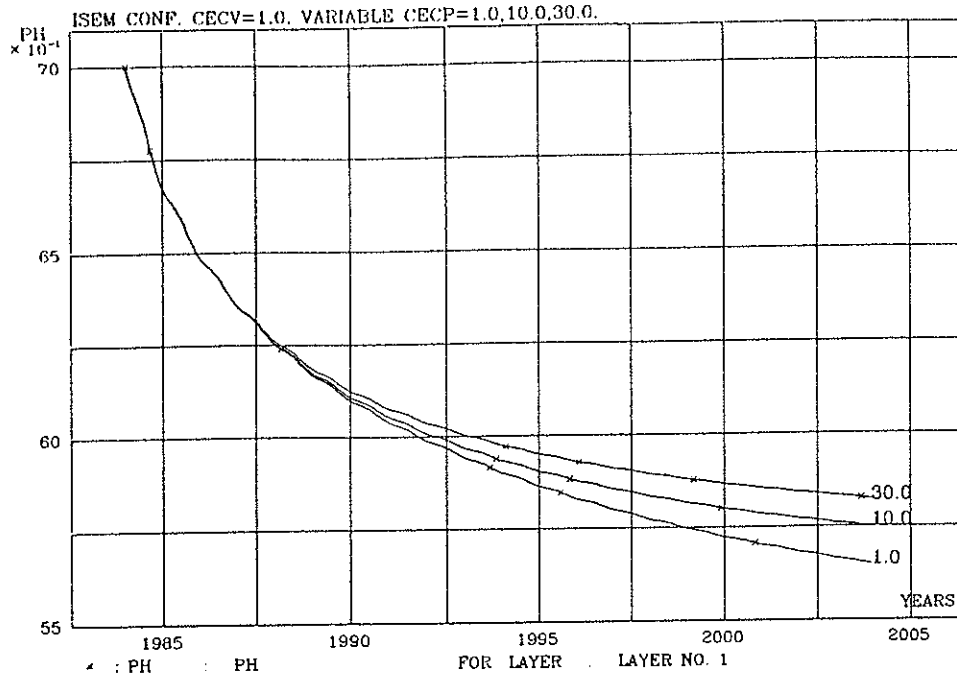


Fig. 22. pH in a test soil when $CEC_v = 1$ meq/100 g and variable CEC_p .

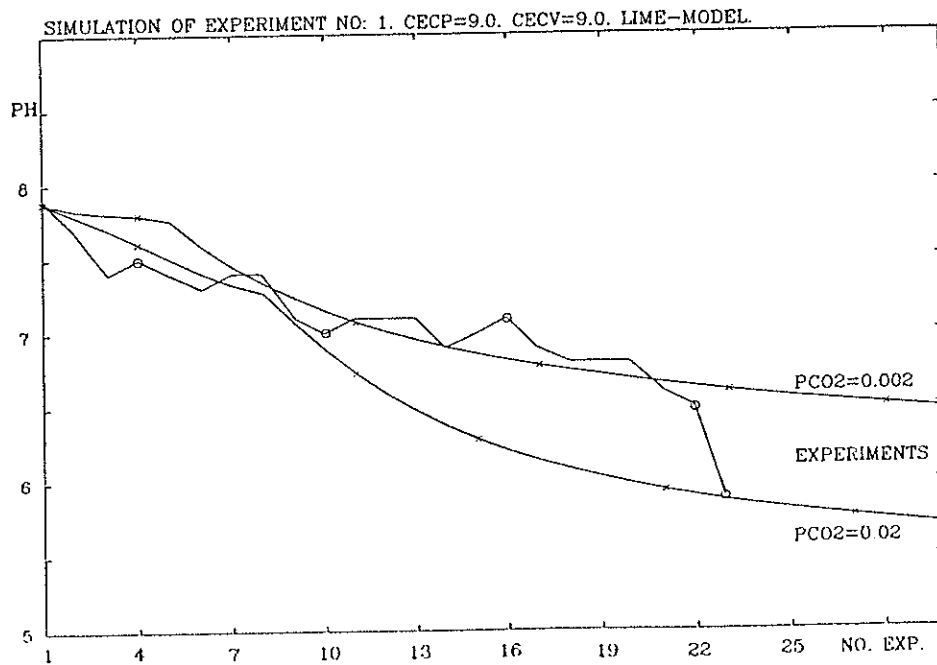


Fig. 23. Simulation of pH in experiments with $pCO_2 = 0.002$ and $pCO_2 = 0.02$ atm.

5. CONCLUSION

Three different models, an atmospheric dispersion model, a soil chemistry model, and a model for ion uptake in crops have been developed. These three models are assembled in a single program, ECCES, where it is possible to run the three models independently or together. The program is very flexible and many input and output options are available. Some databases for areas, cities, plants, crops, soil types, pollutants and meteorology have been created for use with the models.

The program has now reached the stage of development which was planned for the present phase of the project, as illustrated by the scenario calculations in the report. Even so, the models are still to be improved and extended in many areas.

The soil and plant models have been run independently to illustrate their function. The paper presents some calculations which show how results depend on a number of parameters used in some of the submodels. The submodel for atmospheric dispersion has not been tested in this manner. This submodel is considered "proven technology" in the sense it is based on the well-known plume model concept. Thus its accuracy and the permissible domain for use is well understood. This does not mean that the model may not be improved or replaced by other models at a later stage. One of the obvious improvements would be to use deposition velocities dependent on the surface on which deposition takes place.

Calculations of pH in a theoretical test soil showed as expected a pH decrease with time in all soil layers when pH in rainfall was 4.9 and the start pH in soil was 7.0. The decrease was most pronounced in the upper soil layer.

Sensitivity tests were run to show the sensitivity of different parameters. Change in CEC_v (variable cation exchange capacity) within the expected range showed a high buffer effect within the pH range of 5.6 - 7.0, while CEC_p (permanent cation exchange capacity) did not influence pH development very much at high pH. For near neutral soils, determination of CEC_v appears therefore very important for realistic calculations of soil acidification. CEC_p on the other hand influences concentration levels of permanent adsorbed ions in the soil and are important for the buffer effect when pH is 3.8 - 4.5. CEC_p influence the soluble amount of ions and create lower concentrations of dissolved cadmium in the soil water with a high CEC_p value and higher cadmium concentrations with low CEC_p (Christensen et al. 1985).

The same test soil with crops growing on it develops stronger acidification than the same soil without crops. A yearly variation of soil pH is seen as a consequence of released hydrogen ions from the root system. This calculation also showed an increase of soluble cadmium and permanent and variable adsorbed cadmium after 20 years due to cadmium input via rainfall and fertilizer.

It should be stressed again that the results are meant to illustrate how the models work within their theoretical framework and show the sensitivity of some important parameters. Thus one should be careful in drawing quantitative conclusions from the calculations presented. To some extent the models may be used to reveal trends in the development of pollution effects in the environment. However, before more quantitative conclusions can be drawn from the model calculations, more data collections and verification of the models are needed. This will take a considerable part of the future work within this project.

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Title and author(s) ECCES - A MODEL FOR CALCULATION OF ENVIRONMENTAL CONSEQUENCES FROM ENERGY SYSTEMS PREDICTING ION CONCENTRATIONS AND ACIDIFICATION EFFECTS IN TERRESTRIAL ECOSYSTEMS K. Brodersen P.B. Mortensen T. Petersen	Date 1986-10-28
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Abstract (Max. 2000 char.) ECCES is an environmental management model designed to predict environmental impacts from a given energy production scenario in a given geographical area for a period of time. Presently ECCES contains submodels for atmospheric dispersion and deposition of pollutants, soil chemistry and uptake in selected crops. Dispersion is based on a traditional plume model and calculates dispersion of pollutants from many sources (power plants) to counties at Zealand. The soil chemistry model calculates chemical equilibrium between adsorbed and soluble ions in maximum 5 soil layers. CEC is divided between a permanent and a variable cation exchange capacity. Ion uptake in crops is proportional to the equilibrium concentration in the soil water. ECCES is implemented in FORTRAN-77. Inputs are from plant, soil, and crop libraries. Output are prints or datafiles transferable to an independent plot program. Scenario calculations illustrate the capabilities of the program, and sensitivity of some important parameters.	
Descriptors - EDB ACIDIFICATION; COMPUTERIZED SIMULATION; CROPS; DEPOSITION; DISPERSIONS; E CODES; EARTH ATMOSPHERE; ENERGY SYSTEMS; ENVIRONMENTAL IMPACTS; ION EXCHANGE; IONS; NUTRIENTS; PH VALUE; POLLUTANTS; POWER PLANTS; SOIL CHEMISTRY; SOILS; TERRESTRIAL ECOSYSTEMS; TOPOGRAPHY; UPTAKE. Available on request from Risø Library, Risø National Laboratory, (Risø Bibliotek, Forskningscenter Risø), P.O. Box 49, DK-4000 Roskilde, Denmark. Telephone 02 37 12 12, ext. 2262. Telex: 43116, Telefax: 02 36 06 09	

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